WEST Search History

Hide Items | Restore | Clear | Cancel

DATE: Monday, May 10, 2004

Hide?	Set Name	Query	Hit Count
	DB=PGPB,USPT; PLUR=YES; OP=ADJ		
☐	L12	l11 and catechol	0
☐	L11	l6 and l10	6
☐	L10	polymerization inhibitor	8729
☐	L9	l6 and l8	1
☐	L8	cyclohexanecarbonyl chloride	463
☐	L7	cyclohexanevarbonyl chloride	0
☐	L6	l5 and (chlorinat$ or halogenat$)	30
☐	L5	l4 and hydrogenat$	37
☐	L4	l3 and carboxylic acid	93
☐	L3	l2 and acrylic acid	139
☐	L2	l1 and $butadiene	176
☐	L1	cyclohexyl phenyl ketone	539

END OF SEARCH HISTORY

WEST Search History

Hide Items | Restore | Clear | Cancel

DATE: Monday, May 10, 2004

Hide?	Set Name	Query	Hit Count
		DB=PGPB,USPT; PLUR=YES; OP=ADJ	
☐	L3	l2 and acrylic acid	0
☐	L2	l1 and butadiene	11
☐	L1	cycloalkyl aryl ketone$	17

END OF SEARCH HISTORY

```
=> d his

     (FILE 'HOME' ENTERED AT 22:52:08 ON 10 MAY 2004)

     FILE 'CASREACT' ENTERED AT 22:52:27 ON 10 MAY 2004
L1              STRUCTURE UPLOADED
L2            0 S L1
L3           25 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 22:53:40 ON 10 MAY 2004
L4         5256 S ?PHENYL KETONE?
L5         1033 S L4 AND CYCLOHEX?
L6           76 S L5 AND ?DIENE
L7            5 S L6 AND ACRYLIC ACID
L8          204 S L4 AND ?DIENE
L9           13 S L8 AND ACRYLIC ACID
L10          20 S L4 AND DIELS-ALDER?
L11           2 S L10 AND ?CARBOXYLIC ACID
L12         372 S L4 AND ?CARBOXYLIC ACID
L13          16 S L12 AND (HALOGENAT? OR CHLORINAT?)
L14           3 S L13 AND HYDROGENAT?
L15         170 S L12 AND ?CHLORIDE
L16        4994 S POLYMERIZATION INHIBITOR?
L17         385 S L16 AND ?CATECHOL
L18           0 S L12 AND L17
L19           2 S L8 AND ?CATECHOL
L20           1 S L13 AND ?CATECHOL
L21           2 S L6 AND ?CATECHOL
```

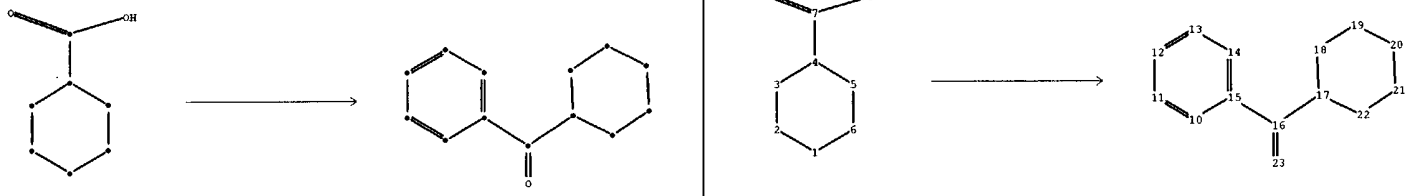
L14 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:307622 CAPLUS
DOCUMENT NUMBER: 140:303405
TITLE: Preparation of cyclohexyl **phenyl** **ketone** from 1,3-butadiene and acrylic acid without purification of intermediates
INVENTOR(S): Ju, Yeong-je; Kim, Jin-eok; Won, Jeong-im; Kan, Tae-yi
PATENT ASSIGNEE(S): Korea Kumho Petrochemical Co., Ltd., S. Korea
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004115499	A2	20040415	JP 2003-201414	20030724
US 2004073068	A1	20040415	US 2003-628800	20030728

PRIORITY APPLN. INFO.: KR 2002-58627 A 20020927

AB Cyclohexyl Ph ketone, useful as an intermediate for photoinitiator 1-hydroxycyclohexyl Ph ketone (no data), is prepared by [2+4] Diels-Alder reaction of 1,3-butadiene with acrylic acid in the presence or absence of solvents, **hydrogenation** of 3-cyclohexene-1-**carboxylic** **acid**, without purification, **chlorination** of the resulting **cyclohexanecarboxylic acid** solution, and without separation of intermediate chloride and byproducts, Friedel-Crafts reaction of the chloride in the same reactor. Acrylic acid was reacted with 1,3-butadiene in the presence of 4-tert-butylcatechol in benzene at 120° for 2 h, **hydrogenated** using Pd/C under 120 psi H at 100°, and **chlorinated** with SOCl2 in benzene under reflux for 1 h to give cyclohexanecarbonyl chloride, which was treated with AlCl3 under reflux for 1 h to give cyclohexyl Ph ketone with ≥99% selectivity at 99% conversion.

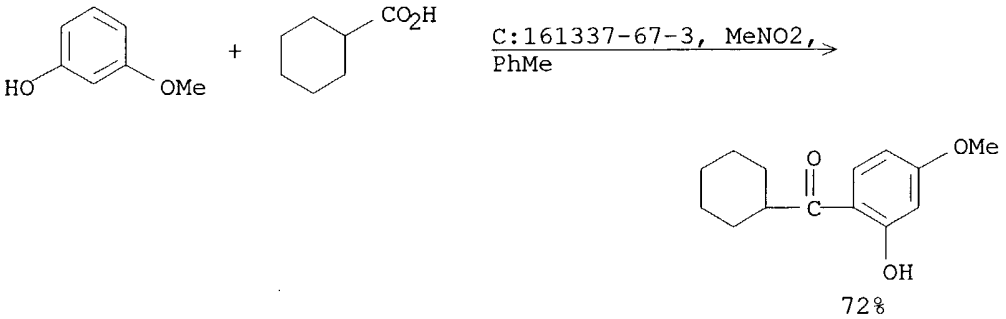
C:\Program Files\Stnexp\Queries\800.str



chain nodes :
7 8 9 16 23
ring nodes :
1 2 3 4 5 6 10 11 12 13 14 15 17 18 19 20 21 22
chain bonds :
4-7 7-8 7-9 15-16 16-17 16-23
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15
17-18 17-22 18-19 19-20 20-21 21-22
exact/norm bonds :
16-23
exact bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 15-16 16-17 17-18 17-22 18-19
19-20 20-21 21-22
normalized bonds :
7-8 7-9 10-11 10-15 11-12 12-13 13-14 14-15
isolated ring systems :
containing 1 : 10 : 17 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:Atom
18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:CLASS
fragments assigned product role:
containing 10
fragments assigned reactant/reagent role:
containing 1

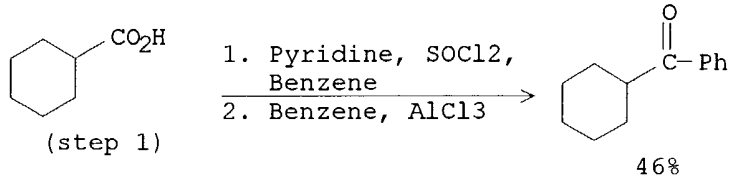
```
L1      STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1              STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


=> s l1
SAMPLE SEARCH INITIATED 22:52:49 FILE 'CASREACT'
SCREENING COMPLETE -     31 REACTIONS TO VERIFY FROM      5 DOCUMENTS

100.0% DONE     31 VERIFIED       0 HIT RXNS                      0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:       286 TO      954
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1 (     0 REACTIONS)

=> s l1 full
FULL SEARCH INITIATED 22:52:54 FILE 'CASREACT'
SCREENING COMPLETE -    600 REACTIONS TO VERIFY FROM    105 DOCUMENTS

100.0% DONE    600 VERIFIED      60 HIT RXNS                     25 DOCS
SEARCH TIME: 00.00.01

L3           25 SEA SSS FUL L1 (    60 REACTIONS)

=> d scan

L3   25 ANSWERS   CASREACT  COPYRIGHT 2004 ACS on STN

TI   Catalytic direct C-acylation of phenol and naphthol derivatives using
     carboxylic acids as acylating reagents

RX(4) OF 4
```




```
NOTE: regioselective


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L3   25 ANSWERS   CASREACT  COPYRIGHT 2004 ACS on STN

TI   Synthesis and structure-activity relationships of potential
```

anticonvulsants based on 2-piperidinecarboxylic acid and related pharmacophores

RX(2) OF 193



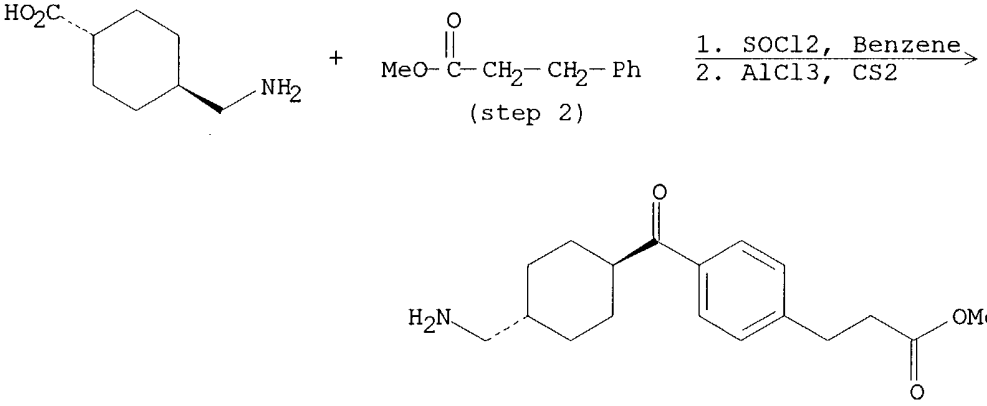
(step 1)

46%

L3 25 ANSWERS CASREACT COPYRIGHT 2004 ACS on STN

TI A facile synthesis of aminocarboxylic acid derivatives, new anti-ulcer agents

RX(8) OF 13 - 2 STEPS

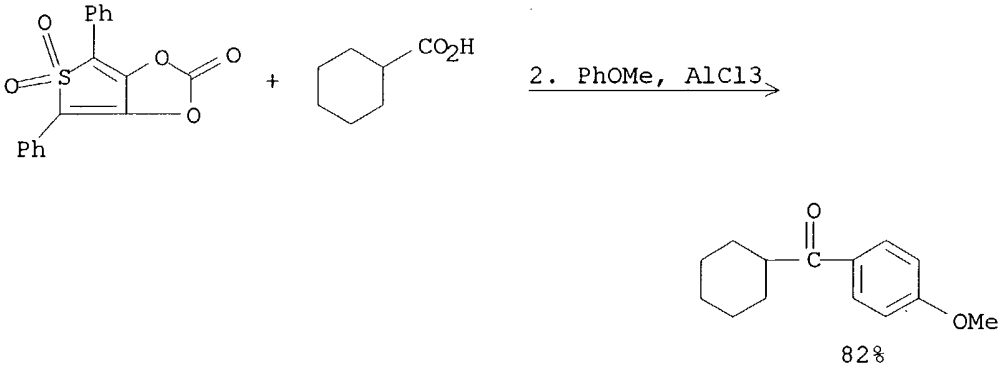


HCl

L3 25 ANSWERS CASREACT COPYRIGHT 2004 ACS on STN

TI 4-Acyloxy-2,5-diphenyl-3-oxo-2,3-dihydrothiophene 1,1-dioxides as acylating agents in the Friedel-Crafts reaction

RX(35) OF 47 - 2 STEPS

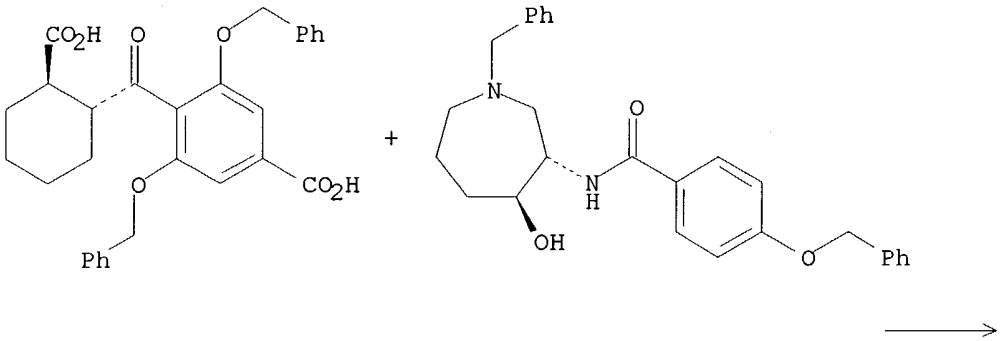


82%

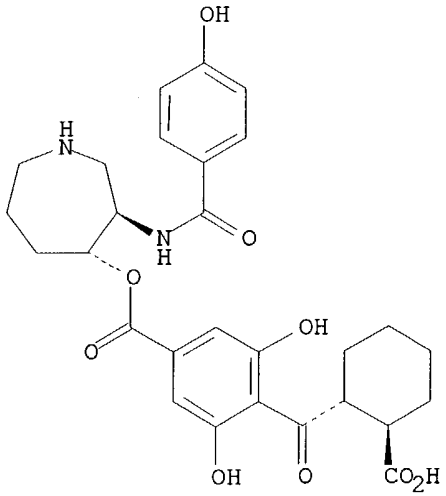
L3 25 ANSWERS CASREACT COPYRIGHT 2004 ACS on STN

TI Synthesis and Protein Kinase Inhibitory Activity of Balanol Analogues with Modified Benzophenone Subunits

RX(77) OF 305



RX(77) OF 305



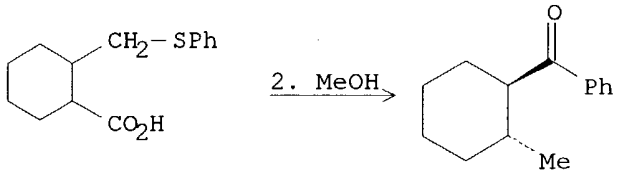
5%

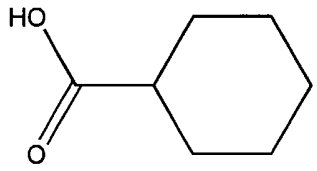
NOTE: general procedure available

L3 25 ANSWERS CASREACT COPYRIGHT 2004 ACS on STN

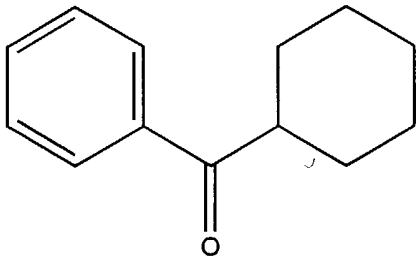
TI Syntheses of 6,6a,7,8,9,10,10a,11-octahydro-11-oxodibenz[b,e]oxepins and 6,6a,7,8,9,10,10a,11-octahydro-11-oxodibenzo[b,e]thiepins

RX(11) OF 14 - 2 STEPS





cyclohexanecarboxylic acid



cyclohexyl phenyl ketone